

Ethylparaben
120-47-8 | DTXSID9022528

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 98.6 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.86e-01

Confidence level: 8.13e-01

Nearest Neighbors from the Training Set

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N-(3-chlorophenyl)-N'-methylurea

Measured: 85.1
Predicted: 101

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N-(3-chloro-4-methylphenyl)-N'-methylurea

Measured: 126
Predicted: 99.6

Image not found

Urea, (3-chloro-4-methoxyphenyl)-

Measured: 100
Predicted: 47.5

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Ethylparaben

Measured: 162
Predicted: 98.6